

1244 **C₃H₆Cl₂**
ED, MM calculations

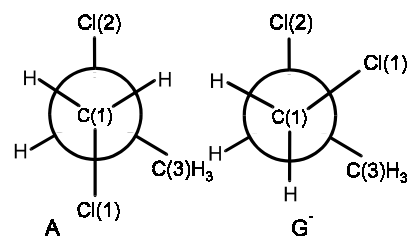
1,2-Dichloropropane

C₁ (A)
C₁ (G⁻)
H₃C-CHCl-CH₂Cl

r_a	$\text{\AA}^a)$	θ_α	$\text{deg}^a)$
C-C	1.519(6)	C(1)-C(2)-C(3) (A) ^{b)}	114.4(16)
C-Cl	1.793(5)	Cl(1)-C(1)-C(2) (A) ^{b)}	111.2(9)
C-H	1.113(12)	Cl(2)-C(2)-C(1) (A) ^{b)}	108.0(11)
		Cl(2)-C(2)-C(3)	109.7(11)
		C(2)-C(1)-H	109.8 ^{c)}
		Cl(1)-C(1)-H	109.0 ^{c)}
		C(1,3)-C(2)-H	109.0 ^{c)}
		C(2)-C(3)-H	110.0 ^{c)}
		ϕ (A) ^{d)}	174(6)
		ϕ (G ⁻) ^{d)}	-58(10)

The molecule exists as a mixture of *anti* A (74(7)%) and *gauche* G⁻ (26(7)%) conformers. Local symmetries C_{3v}, C_s and C_s were assumed for the C-CH₃, CH₂Cl and C-CH-C groups, respectively. The lengths of all the C-H bonds and the two C-Cl bonds and the Cl-C(2)-C(3) angles for all the conformers were assumed to be equal.

The nozzle was at 26 °C



^{a)} Twice the estimated standard errors.

^{b)} Conformational differences were fixed at the values from molecular mechanics calculations.

^{c)} Values from molecular mechanics calculations.

^{d)} Torsion angle Cl-C-C-Cl.

Schei, S.H., Stølevik, R.: J. Mol. Struct. **128** (1985) 171.